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A PARAMETRIC DESCRIPTION OF A SKEWED PUFF IN THE DIABATIC SURFACE LAYER

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Abstract. The spreading of passive material from an instantaneous ground source in the stable, neutral, and unstable surface layers is parameterized in a form appropriate for use with an operational puff diffusion model.

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FORMULATION AND EXPERIMENTAL EVALUATION OF AN OPERATIONAL PUFF DIFFUSION MODEL

submitted to the Technical University of Denmark together with the reports Risø-R-475 and Risø-R-479 in partial fulfilment of the requirements for the degree of lic.techn. (Ph.D.).

Professor K. Refslund acted as responsible supervisor and mag.scient. L. Kristensen functioned as advisor. Professor E. Eliasen was appointed external examiner.

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CONTENTS

1. INTRODUCTION

Spatial and temporal variations in meteorological conditions, including nonuniform topographical features, lake or sea-breeze circulation, and urban heat-island effects have during the past years given a bases for several puff diffusion model proposals: Roberts et al. (1970), Lamb and Neiburger (1971), Start and Wendell (1974), Ludwig et al. (1977), Sheih (1978), Mikkelsen (1979) and Mikkelsen et al. (1980). In all these the release of pollutant from the source has been treated as a series of puffs emitted successively into the atmosphere. The concentration distribution of the individual puffs have hitherto been assumed to be Gaussian along the vertical as well as the horizontal axes. The model of Sheih (1978), however, included also the effect of wind shear and buoyant plume rise.

In analogy to diffusion from a continuous source, the vertical diffusion from an instantaneous source is especially influenced strongly by the effect of atmospheric stability. This applies with respect to both the spreading of the cloud and shape of the vertical distribution function.

Therefore, an operational puff model algorithm is proposed here which takes into account the effect of stability of the following quantities:

1) the vertical dispersion of the cloud,
2) the shape of the vertical concentration distribution, and
3) the diffusion associated with wind shear.

2. THEORY

2.1. Parameterization of vertical puff diffusion

By assuming identity of eddy diffusivities of passive material K_z and of heat K_h, Chaudhry and Meroney (1973) studied the effect of stability on the instantaneous vertical diffusion from a ground-level point source. Nieuwstadt and van Ulden (1978) showed that this identification could lead to an overprediction of the vertical spread from a continuous source under stable conditions and obtained better agreement with the Prairie Grass data with $K_z = \alpha_o K_m$, where K_m is the eddy diffusivity for momentum, and α_o is a constant which is equal to the ratio K_h/K_m in neutral stratification. In the present model K_z is set equal to K_h, but with the remark above in mind; later experimental findings may make a change to $\alpha_o K_m$ appropriate. From a mathematical point of view, however, this will amount to only a trivial substitution.

The Lagrangian similarity hypothesis considers the problem of diffusion of an ensemble of marked particles of fluid, released individually from a fixed ground source at time t = 0. Each such released fluid particle will occupy a different position at time t after the release, and $\bar{x}(t)$ and $\bar{z}(t)$ denotes the ensemble-averaged longitudinal and vertical displacements relative to the source position at time t. In a homogeneous and stationary flow field, such a diffusion may be like that of a cloud of marked particles or a puff, released from a ground source at one instant (Pasquill, 1966) (see Fig. 1). This is described by the distribution of concentration C(x,y,z,t) $[\mathrm{kg\ m^{-3}}]$ at a point (x,y,z) at time t, which for a cloud of passive substance may be obtained from the diffusion equation in a plane homogeneous turbulent shear layer

$$\frac{\partial C}{\partial t} + \bar{u}(z)\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial C}{\partial y}\right) . \qquad (2.1)$$

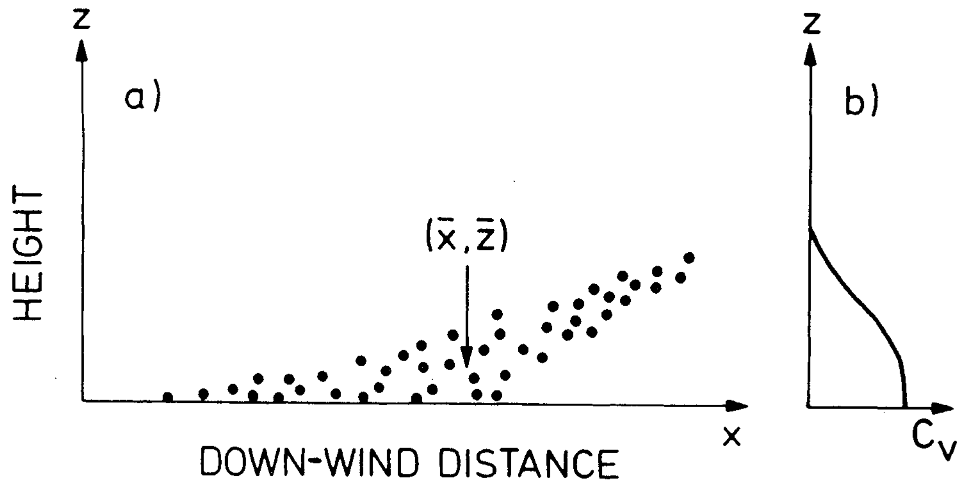

Fig. 1. a) Diffusion of a number of particles released at $x = 0$ at time $t = 0$. The instantaneous position of the centre of mass of the cloud $(\bar{x},\bar{z})$ is indicated by the head of the arrow. b) The corresponding instantaneous vertical particle distribution $C_V(z,t)$.

The longitudinal diffusion term is neglected, since this can be assumed to be much smaller than the corresponding term $\bar{u}(\partial C/\partial x)$. The parameters K_y and K_z are the eddy diffusivities of matter in the y- and z-directions, respectively. The downwind direction is denoted by x, and $\bar{u}(z)$ is the mean wind speed as a function of height z. The dependence of C on y in the above equation can be integrated out to give

$$\frac{\partial \tilde{C}}{\partial t} + \bar{u}(z)\frac{\partial \tilde{C}}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial \tilde{C}}{\partial z}\right) \qquad (2.2)$$

where $\tilde{C}(x,z,t) = \int_{-\infty}^{\infty} C(x,y,z,t)dy$ $[\mathrm{kg\ m^{-2}}]$ is the concentration that would arise from an infinitely long, crosswind-oriented line source. If the total amount of substance in the cloud is unity, the instantaneous position of its centre of mass will be given by

$$\bar{x}(t) = \int_{0}^{\infty}\int_{-\infty}^{\infty} x\,\tilde{C}(x,z,t)\,dxdz \qquad (2.3)$$

$$\bar{z}(t) = \int_{0}^{\infty}\int_{-\infty}^{\infty} z\,\tilde{C}(x,z,t)\,dxdz \qquad (2.4)$$

Multiplying Eq. (2.2) by z and x, respectively, a subsequent integration over all values of x and z yields for times t > 0

$$\frac{d\bar{z}}{dt} = \int_{o}^{\infty} z \frac{\partial}{\partial z}\left(K_z \frac{\partial C_V}{\partial z}\right) dz \tag{2.5}$$

$$\frac{d\bar{x}}{dt} = \int_{o}^{\infty} \bar{u}(z)\, C_V\, dz \tag{2.6}$$

where $C_V = \int_{-\infty}^{\infty} \tilde{C}\,(x,z,t)\, dx\ [kg\ m^{-1}]$ denotes the average number of particles between the heights z and z + dz (see again Fig. 1). An equation for the vertical distribution of C_V can be obtained by integrating Eq. (2.2) with respect to x, as

$$\frac{\partial C_V}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C_V}{\partial z}\right) \tag{2.7}$$

The important relationship in Eqs. (2.5) and (2.6) for the centre of mass coordinates of the puff can now be evaluated for termally stratified flow if $K_z(z)$ and $C_V(z,t)$ are known. Based on the Monin-Obukhov similarity hypothesis, the assumed diffusivity for contaminant in the surface layer now reads

$$K_z = \frac{k\ u_* z}{\phi_h(\frac{z}{L})} \tag{2.8}$$

where k is von Karman's constant (0.35), u_* the friction velocity and $\phi_h(z/L)$ is the dimensionless temperature gradient, which is a function of the ratio of the height z to the Monin-Obukhov length L, only.

The diffusion equation (2.7) can be solved analytically when this eddy diffusivity is approximated by a power-law profile $K_z = K_1\, z^n$. For such a profile the solution of Eq. (2.7) is (Sutton, 1953)

$$C_V = \frac{a}{\bar{z}} \exp[-(bz/\bar{z})^q] , \tag{2.9}$$

where

$$q = 2-n$$
$$a = q\Gamma(2/q)/\Gamma^2(1/q)$$
$$b = \Gamma(2/q)/\Gamma(1/q),$$

and where Γ is the gamma function. The power n may be regarded as an index of stability. Estimates for n and for $q = 2-n$ can be obtained by a procedure suggested by Klug (1963) to fit a power law representation to the original K_z-profile. This procedure yields

$$n = \{d\log K_z/d\log z\}_{z=\bar{z}} \tag{2.10}$$

Businger (1973) gives the dimensionless temperature gradient

$$\phi_h = 0.74(1 + 6.3\ z/L) \qquad \text{for } 1/L \geq 0 \tag{2.11}$$

and

$$\phi_h = 0.74(1 - 9\ z/L)^{-1/2} \qquad \text{for } 1/L \leq 0 \tag{2.12}$$

The corresponding powers obtained on the basis of Eq. (2.9) and with $q = 2-n$ are

$$q = \frac{0.74}{0.74+4.7\ \bar{z}/L} \qquad \text{for } 1/L \geq 0 \tag{2.13}$$

$$q = \frac{1-13.5\ \bar{z}/L}{1-9\ \bar{z}/L} \qquad \text{for } 1/L \leq 0 \tag{2.14}$$

For neutral conditions $q = n = 1$, and the vertical distribution function of the puff then takes the simple form

$$C_V = \frac{1}{\bar{z}} \exp[-z/\bar{z}] \tag{2.15}$$

This brings out the important difference between a continuously released plume and an instantaneous puff. In contrast to the result in Eq. (2.15), dispersion from a continuous ground level source, obtained from measurements at a fixed point in space, typically fits to the power $q \approx 1.3$ under neutral conditions.

For a limited range of the stability index q around 1, Chaudhry and Meroney (1973) reduced the expressions on the right-hand side of Eqs. (2.5) and (2.6), to the approximate form, which will be used in the following:

$$\frac{d\bar{z}}{dt} \approx k u_* \phi_h^{-1}(\bar{z}/L) \tag{2.16}$$

and

$$\frac{d\bar{x}}{dt} \approx \bar{u}(\bar{z}) - 1.44\ u_* \tag{2.17}$$

The mean wind speed over local homogeneous terrain, as function of height z and the surface roughnes parameter z_o, is here also taken from Businger (1973)

$$\bar{u}(z) = (u_*/k)\left[\ell n(z/z_o) - \Psi(z/L)\right] \tag{2.18}$$

where, for $1/L \geq 0$

$$\Psi = -4.7\ z/L \tag{2.19}$$

and for $1/L \leq 0$

$$\Psi = 2\ \ln\left[(1+x)/2\right] + \ln\left[(1+x^2)/2\right] - 2\ \tan^{-1}(x) + \pi/2 \tag{2.20}$$

$$x = (1 - 15\ z/L)^{1/4}$$

The individual released puffs, however, must be advected, not by the mean wind $\bar{u}$, but by a time series of the non-stationary wind field $\underline{V}$. This time series will therefore in general be a function of the downwind position x, the time since releases t, and the wind field averaging time t_{av}. For use with microscale and mesoscale puff models, the wind field $\underline{V}$ is obtainable by an "objective" wind field analysis, based on simultaneous measurements of wind speed and directions from a network of meteorological towers (see, e.g. L.L. Wendell, 1970). Depending on the size of the puffs, the averaging time t_{av}, (which also is used conveniently in computer simulations as the basic time step for the puff advection), must be chosen to be short enough to ensure that sufficient temporal variation will be present in the advecting wind field.

If $\bar{u}(z_m)$ represents the speed of the wind vector $\underline{V}$ during the time interval from t to t + t_{av}, at the height z_m and at the horizontal position (x,y), then the wind speed for advection of the puffs in that horizontal position, and over the time period from t to t + t_{av} is calculated by means of

$$\bar{u}_r(z) = \bar{u}(z_m) \cdot \left[\frac{\ln(z/z_o) - \Psi(z/L)}{\ln(z_m/z_o) - \Psi(z_m/L)} \right] , \qquad (2.21)$$

assuming that $|\underline{V}|$ also follows the usual mean wind profile. For use with an operational puff diffusion algorithm, the set of equations (2.9), (2.16) and (2.17) determine together with the wind field in Eq. (2.21) the shape of the vertical distribution function of the puffs as well as their downwind position as function of stability and travel time. However, these equations are based on approximations. It is assumed that K_z can be represented by a power law of the variable z, and their validity must therefore be based on a comparison with a numerical solution of the diffusion equation (2.7) with the eddy diffusivity K_z as specified by Eqs. (2.8), (2.11) and (2.12).

2.2. Numerical solutions

The boundary conditions applied to a numerical solution of the diffusion equation (2.7) is

$$K_z \frac{\partial C_V}{\partial z} = 0 \qquad \text{for } z = z_o \tag{2.22}$$

and

$$K_z \frac{\partial C_V}{\partial z} = 0 \qquad \text{for } z \to \infty\,. \tag{2.23}$$

They state that the vertical mass flux at the ground and at infinity must vanish. The initial vertical concentration distribution function was chosen to be Gaussian with maximum concentration at ground level and a standard deviation equal to $2z_o$. Except for very small values of the dimensionless time u_*t/L, the numerical results were found to be insensitive to the specific form of the initial distribution.

With the boundary and initial conditions as described, the diffusion equation in non-dimensional form is

$$\frac{\partial C_V}{d(u_*t/L)} = k \frac{\partial}{\partial \eta} \left(\eta \phi_h^{-1}(\eta) \frac{\partial C_V}{\partial \eta} \right), \tag{2.24}$$

where $\eta = z/L$, was solved numerically by a finite difference scheme proposed by Keller (1971) and implemented for use in the investigations by S.E. Gryning et al. (1982). During numerical calculations, the conservation of mass was continuously verified by integration of the distribution C_V in the vertical direction. As also found by Gryning et al. (1982), errors were maintained below 1%.

2.3. Results

Comparisons were made between the numerical solutions of Eq. (2.24) and the approximation suggested in Section 2.1. Figure 2 compares the variation of the mean height of the puff $\bar{z}$ as a function of its non-dimensional travel time $u_*t/|L|$. The suggested approximation in Eq. (2.16) is seen to model very well the variation of $\bar{z}$ based on the numerical integration of the diffusion equation, together with the definition of $\bar{z}$ in Eq. (2.4).

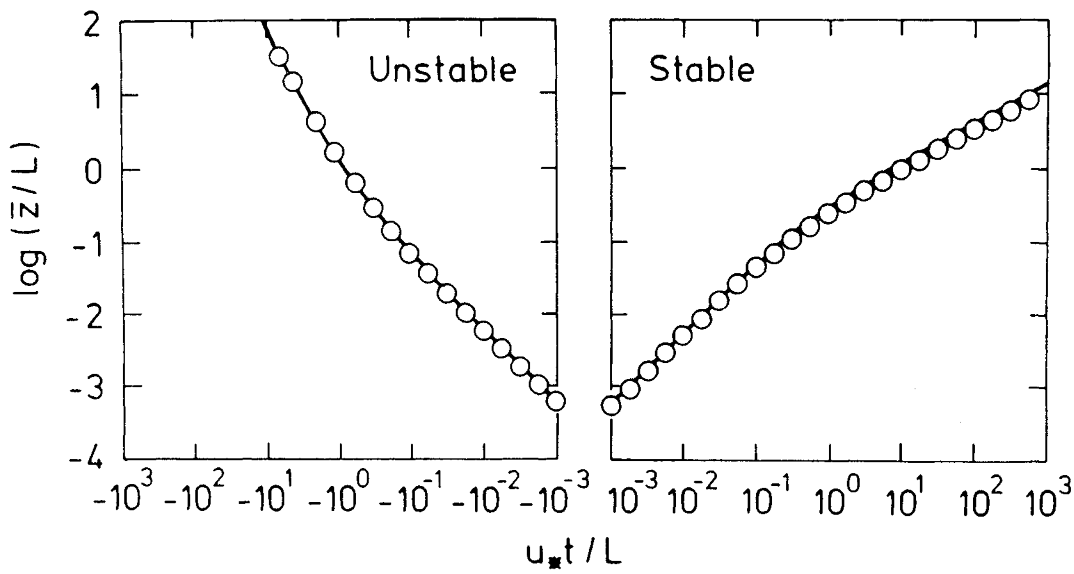

Fig. 2. Dimensionless mean puff height $\bar{z}/L$ as function of the dimensionless travel time u_*t/L. The curve shows the approximation suggested in Eq. (2.16). The open circles represent the result of the numerical solution of the diffusion equation (2.24), together with the definition of $\bar{z}$, Eq. (2.4).

In the limit for small times $tu_*/|L| \to 0$, which for fixed t corresponds to near neutral stratification, the approximate solution is $\bar{z} = ku_*t$. Based on the ϕ_h-functions chosen in Eqs. (2.11) and (2.12) the asymptotic values for the large time limits are, for the stable and the unstable stratification: $\bar{z} \propto t^{1/2}$ and $\bar{z} \propto t^2$, respectively. Dimensional analysis for the z-less (very stable) stratification yields accordingly $\bar{z} \propto t^{1/2}$, but in the unstable atmosphere, for which case convective scaling applies and $\phi_h \simeq (z/|L|)^{-1/3}$, dimensional analysis yields $\bar{z} \propto t^{3/2}$. The different asymptotic form found here, $\bar{z} \propto t^2$, results as a consequence of the empirical functional form observed for ϕ_h (Eq. (2.12)) in the convective limit. This discrepancy is deemed to be insignificant except under the most unstable conditions, in which case K-theory is known to be inapplicable in any event.

Figure 3 shows the exponent q as function of the non-dimensional travel time of the cloud, u_*t/L. The dots were obtained by least-square fitting to the analytical function described by Eq. (2.9) of the vertical concentration profiles; the latter are obtained from the numerical solution of Eq. (2.24). The fittings

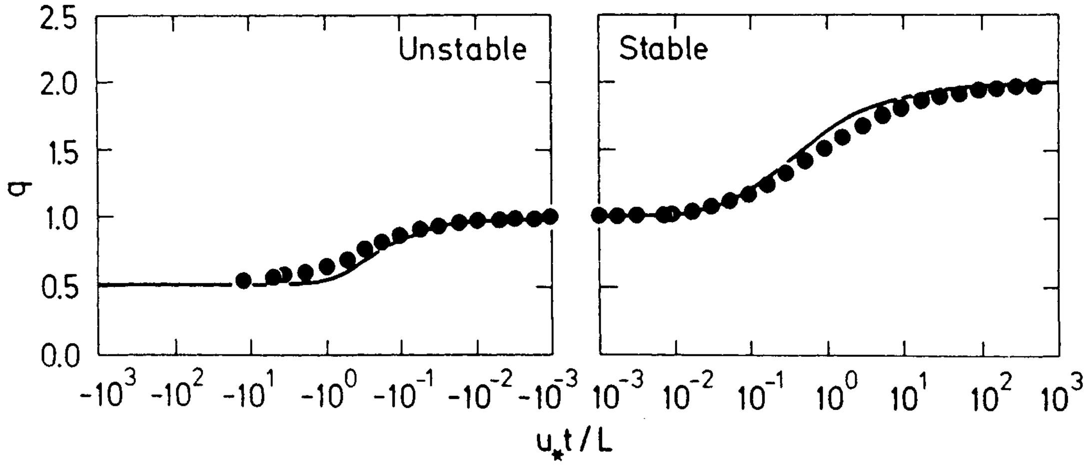

Fig. 3. The shape factor q, as function of non-dimensional travel time u_*t/L. The curves show the analytical approximation suggested in Eqs. (2.13) and (2.14). Dots represent a least-square fitting of the analytical function described by Eq. (2.9) to C_y obtained from the numerical solution of Eq. (2.24).

were accomplished from the ground up to the level where the concentration constituted 5% of the maximum value by forcing the analytical function through the concentration at ground level. The relative root-mean-square difference turned out to be lower than 0.1% for the parameter interval $u_*t/|L| < 10^{-2}$. Under stable conditions the maximum error, of the order ~ 2%, was found for $u_*t/L \simeq 5\cdot 10^{-1}$. Correspondingly, the maximum error under unstable conditions was of the order 3% and was found with $u_*t/L \simeq -5\cdot 10^{-1}$. The very low root-mean-square error found for $u_*t/|L| < 10^{-2}$ reveals that an exponential distribution function is an exact solution to the diffusion equation under neutral conditions, since n and hence q in Eq. (2.9) equals unity, when $1/|L| \sim 0$. The curve in Fig. 3 shows the analytical approximation suggested in Eq. (2.13) for stable and in Eq. (2.14) for unstable conditions.

For all practical purposes, these curves are found to approximate the numerical solution very well. The variation in the shape parameter q with travel time is quite pronounced. Under stable conditions, the initially small, exponentially distributed cloud ultimately becomes Gaussian, i.e. q = 2. Under unstable conditions, on the other hand, the ultimate vertical distribution function becomes quite stretched ($q \approx 0.5$). This result shows a significant difference from the Gaussian vertical distribution usually assumed with puff models.

3. THE MODEL

3.1. Horizontal puff diffusion

So far we have been dealing exclusively with the vertical dis- distribution function of the particles, which was defined in the previous paragraph as

$$C_V(z) = \iint_{-\infty}^{\infty} C(x,y,z)\, dxdy \tag{3.1}$$

In order to calculate the entire concentration field $C(x,y,z)$, however, the distribution function of particles in the two horizontal directions will also have to be resolved. We therefore consider the part of the cloud which is confined to the small vertical interval Δz, centered around the horizontal plane $z = h$. The horizontal distribution function of the particles at this height C_H, when normalized, is then given by the expression

$$C_H(x,y,h) = C(x,y,h)\Delta z / \iint_{-\infty}^{\infty} C(x,y,h)\Delta z\, dxdy \tag{3.2}$$

In this way the mean horizontal coordinates $\bar{x}$ and $\bar{y}$ of the particles in the small interval Δz about $z = h$ become

$$\bar{x}_z = \iint_{-\infty}^{\infty} x\, C_H(x,y,h)\, dxdy \tag{3.3 a}$$

$$\bar{y}_z = \iint_{-\infty}^{\infty} y\, C_H(x,y,h)\, dxdy \tag{3.3 b}$$

In contrast to dispersion taking place in the vertical direction in the atmosphere, horizontal dispersion of a cloud can, with some justification, be claimed to proceed in a homogeneous field of turbulence. This is true at least as long as the horizontal extent of the individual puffs, but not the entire plume, is small compared with the distances over which inhomogeneity of the turbulent field occurs. In this case, the ensemble-averaged horizontal distribution function of the cloud is well taken to be Gaussian. This can be derived from theoretical considerations (e.g. Batchelor (1952)) and also seen from experimental evidence (e.g. Sullivan (1971)). Also Yang and Meroney (1972, 1973) measured at fixed x and z the centerline concentration as a function of time from a surface-released cloud in a wind tunnel boundary layer. Wilson (1981) compared their measured skewed distribution with a Gaussian distribution and concluded that the errors induced by applying a symmetric Gaussian distribution to the along-wind diffusion (at fixed height) could be expected to be small compared with the uncertainties in estimating the corresponding along-wind standard deviation σ_x.

In the following reference will be changed from the fixed (absolute) coordinate system (x,y,z) to the frame of reference $(\bar{x}_o, \bar{y}_o, 0)$ moving with the centeroid of the cloud at height $z = z_o$. In this moving frame we define a relative Cartesian coordinate system as

$$\begin{aligned} \tilde{x} &= x - \bar{x}_o \\ \tilde{y} &= y - \bar{y}_o \\ \tilde{z} &= z \end{aligned} \qquad (3.4)$$

The mean horizontal position of the particles at the height z in this relative frame is also defined as

$$\begin{aligned} \bar{\tilde{x}}_z &= \bar{x}_z - \bar{x}_o \\ \bar{\tilde{y}}_z &= \bar{y}_z - \bar{y}_o \end{aligned} \qquad (3.5)$$

In this relative frame of reference, an assumed horizontal Gaussian particle distribution function simply reads

$$C_H(\tilde{x},\tilde{y},\tilde{z}) = \frac{1}{2\pi\sigma_x\sigma_y} \exp\left\{-\frac{1}{2}(\tilde{x}-\overline{\tilde{x}}_z)^2/\sigma_x^2 - \frac{1}{2}(\tilde{y}-\overline{\tilde{y}}_z)^2/\sigma_y^2\right\} \tag{3.6}$$

where σ_x and σ_y are the streamwise and lateral standard deviations, respectively, of the cloud at the fixed height z = h.

Suppose now that σ_x, σ_y, $\overline{\tilde{x}}_z$ and $\overline{\tilde{y}}_z$ are known functions of height z and time t. Then, as a consequence of the assumed form of the horizontal distribution function, Eq. (3.6), the entire three-dimensional concentration field of the cloud must be given by

$$C(\tilde{x},\tilde{y},\tilde{z}) = C_V(\tilde{z})\cdot C_H(\tilde{x},\tilde{y},\tilde{z}) \tag{3.7}$$

Note that the marginal distribution C_V is retrieved simply by integrating the right-hand side over a horizontal plane.

3.2. Horizontal turbulent spread, σ_x and σ_y

In past dispersion studies (e.g. Pasquill, 1974) plume and puffs have shown different dispersion characteristics. While the spread of a plume as measured by the horizontal standard diviation of the concentration distribution initially tends to grow proportional to the downwind distance x, and ultimately proportional to the square root of this distance, the characteristics of puff dispersion have shown a different behaviour. In particular, by examining data from smoke puffs Gifford (1957) found the existence of two predicted (Batchelor, 1952) growing regimes for their lateral standard deviation σ_y. Initially, σ_y^2 was found to increase proportionally with x^2 but then an intermediate regime follows, where σ_y^2 grows proportional to the third power of the downwind distance. Ultimately, when the lateral extent of the puff becomes large relative to the lateral length scale of the turbulence, the spreads of a puff and plume become identical.

In contrast to dispersion characteristics available for plumes under various atmospheric conditions, corresponding formulas for puff growth are still relatively sparse.

For use within the atmospheric surface layer and for downwind distances not exceeding ~ 5000 meters, Pasquill (1974) suggested the following expression, supported by the theory of Smith and Hay (1961):

$$\sigma_y = 0.22ix \qquad (3.8)$$

where i is the intensity of the turbulence, defined as $i = (\overline{u'^2} + \overline{v'^2} + \overline{w'^2})^{1/2}/\bar{u}$. As a practical working approximation, i can be estimated from the crosswind eddy velocity, $\overline{v'^2}$, alone. With good approximation the quantity $(\overline{v'^2})^{1/2}/\bar{u}$ is equal to the root-mean-square value of the angular response of a sensitive vane, $i_\theta = (\overline{\theta'^2})^{1/2}$. In his comparison, Pasquill (1974) found reasonably good experimental agreement with Eq. (3.8) by setting $i \simeq 2i_\theta$ in neutral and unstable stratifications and $i = i_\theta$ in the most stable stratifications. It should be mentioned that the theoretical analysis by Chatwin (1968) leads to a puff expansion which close to the ground in a logarithmic surface layer profile reads $\sigma_x = 0.596\, u_* t/k$, applicable in the limit for large diffusion times. Setting $u_*/k \simeq (\overline{u'^2})^{1/2}$ from Businger (1973) and $i \approx 3(\overline{u'^2})^{1/2}/\bar{u}$, this becomes almost equivalent to Eq. (3.8). Here, the spread σ_x is a function of the travel time t of the puff rather than a function of the downwind distance x as in Eq. (3.8). In the present model, use will be made of Eq. (3.8) at short distances because of its experimental validation. For diffusion in the troposphere at distances greater than about 5000 meters, the formula given by Gifford (1982) can be recommended,

$$\Sigma_y^2 = T-(1-e^{-T}) - (c/2)(1-e^{-T})^2 \qquad (3.9)$$

Here, $\Sigma_y^2 = \sigma_y^2/(2\overline{v'^2}t_L^2)$, $T = t/t_L$, and c is a constant close to unity (0.9955)*). The quantity t_L is the integral time scale of

*) Reference is made to the original work (Gifford, 1982) for a more complete discussion.

the turbulence. Note that both of these formulas (Eqs. (3.8) and (3.9)) apply to lateral spread only, and are independent of height z. Further, a local horizontal homogeneity will be assumed together with the relation $\sigma_x = \sigma_y$.

3.3. Wind shear effect

As shown for instance by Chatwin (1968), the horizontal spread of a cloud is strongly influenced by the interaction of wind shear and vertical diffusivity, except under the most unstable conditions. By assuming that the wind shear is approximatively constant across the cloud, it is possible, as also suggested by Sheih (1978), to incorporate the shearing effect in the cloud by the relations

$$\overline{\tilde{x}}_z = \zeta\tilde{z} \tag{3.10}$$

and

$$\overline{\tilde{y}}_z = \xi\tilde{z} \tag{3.11}$$

Here the values of the variables ζ and ξ will be calculated by following the horizontal mean position of two tracer particles (1) and (2), displaced respectively above and below the mean height $\bar{z}(t)$ by the constant fraction F of the mean height of the cloud

$$F = (z_1-z_2)/2\bar{z}. \tag{3.12}$$

The vertical positon of the particles (1) and (2) are, respectively, z_1 and z_2. With the two particles initially at the downwind position $x_1 = x_2 = 0$, the variable ζ which determines the along-wind shearing of the puff as function of time and stability, is calculated by (cf. Fig. 4)

$$\zeta = \frac{x_1-x_2}{\bar{z}} = \frac{1}{\bar{z}}\int_o^t (\bar{u}_r\{\bar{z}(1+F)\} - \bar{u}_r\{\bar{z}(1-F)\})d\tau \tag{3.13}$$

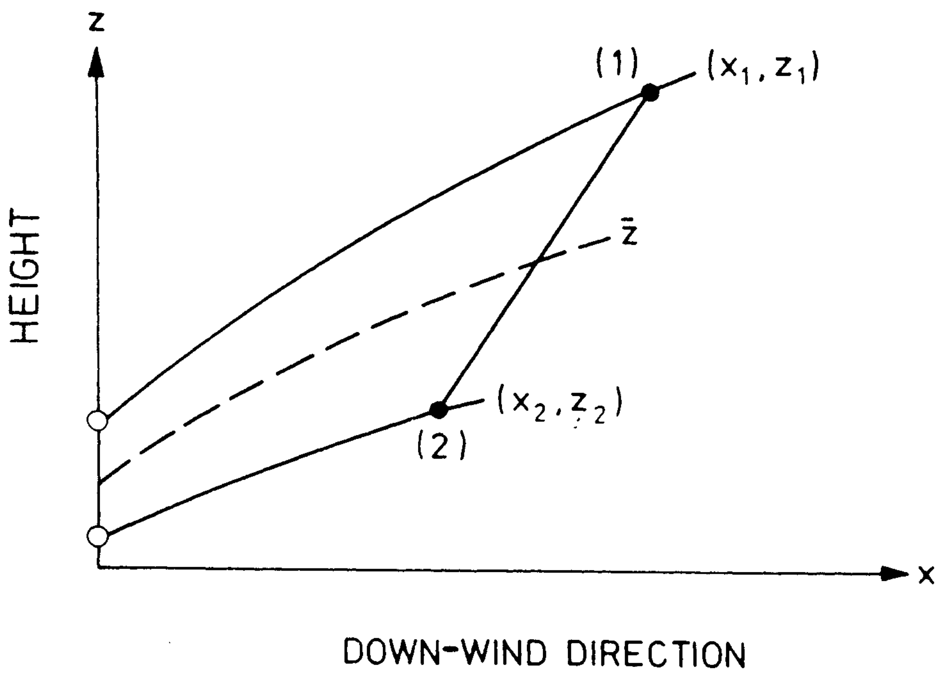

Fig. 4. Two tracer particles (1) and (2) displaced vertically by a constant fraction $F = (z_1-z_2)/2\bar{z}$ of the mean height $\bar{z}$ of the cloud.

Equivalently, the variable ξ determining the crosswind shearing of the puff is calculated by

$$\xi = \frac{y_1-y_2}{\bar{z}} = \frac{1}{\bar{z}} \int_0^t \bar{v}_r\{\bar{z}(1+F)\} - \bar{v}_r\{\bar{z}(1-F)\}\, d\tau \qquad (3.14)$$

Analogously, y_1 and y_2 are the crosswind position of the two particles (1) and (2), and $v_r(z)$ is the short-term averaged (averaging time = t_{av}, cf. Eq. 2.21) mean lateral windspeed as a function of height.

In analogy to $u_r(z)$, $v_r(z)$ is obtainable also from the wind field $\underline{V}$ from an equation similar to Eq. (2.21), but in contrast to $u_r(z)$ the mean value of $v_r(z)$, averaged over many advection steps, is by definition equal to zero.

The only remaining parameter responsible for the shearing effect of the puff is the constant F. Its determination will be postponed until we have investigated some statistical properties of the entire concentration distribution of the cloud in the next section.

3.4. Statistical properties of the cloud distribution function

From the Eqs. (3.4) and (3.5), the 3-dimensional particle distribution function of the skewed puff now reads

$$C(\tilde{x},\tilde{y},\tilde{z})$$

$$= \frac{a}{2\pi\sigma_x\sigma_y\,\bar{z}} \exp\left\{-\frac{1}{2}(\tilde{x}-\zeta\tilde{z})^2/\sigma_x^2) - \frac{1}{2}(\tilde{y}-\xi\tilde{z})^2/\sigma_y^2 - \left(\frac{b\tilde{z}}{\bar{z}}\right)^q\right\} \tag{3.15}$$

With this distribution function, it is relatively simple to derive the following statistical relations for the cloud:

1) Centre of mass

$$\bar{\tilde{x}} = \zeta\tilde{z} \tag{3.16}$$

$$\bar{\tilde{y}} = \xi\tilde{z} \tag{3.17}$$

2) Total horizontal variance, $\Sigma_x^2 \equiv \overline{x^2} - \bar{x}^2$ and $\Sigma_y^2 = \overline{y^2} - \bar{y}^2$

$$\Sigma_x^2 = \sigma_x^2 + \frac{\Gamma(\frac{1}{q})\,\Gamma(\frac{3}{q}) - \Gamma(\frac{2}{q})}{\Gamma(\frac{2}{q})}\,\zeta^2\,\bar{z}^2 \tag{3.18}$$

$$\Sigma_y^2 = \sigma_y^2 + \frac{\Gamma(\frac{1}{q})\,\Gamma(\frac{3}{q}) - \Gamma(\frac{2}{q})}{\Gamma(\frac{2}{q})}\,\xi^2\,\bar{z}^2 \tag{3.19}$$

3) Total vertical variance, $\Sigma_z^2 = \overline{z^2} - \bar{z}^2$

$$\Sigma_z^2 = \frac{\Gamma(\frac{1}{q})\,\Gamma(\frac{3}{q}) - \Gamma(\frac{2}{q})}{\Gamma(\frac{2}{q})}\,\bar{z}^2 \tag{3.20}$$

4) Correlation coefficient $\rho_{xz} \equiv \overline{xz}/\Sigma_x\Sigma_z$ and $\rho_{yz} = \overline{yz}/\Sigma_y\Sigma_z$

$$\rho_{xz} = 1/\left\{1 + \frac{\sigma_x^2}{(\Gamma_{123}-1)\zeta^2\bar{z}^2}\right\}^{1/2} \tag{3.21}$$

$$\rho_{yz} = 1/\left\{1 + \frac{\sigma_y^2}{(\Gamma_{123}-1)\xi^2\bar{z}^2}\right\}^{1/2} \tag{3.22}$$

where $\Gamma_{123} \equiv \Gamma(1/q)\cdot\Gamma(3/q)/\Gamma^2(2/q)$. Note especially that for $q = 1$, $\Sigma_z^2 = \bar{z}^2$ and for $q = 2$, $\Sigma_z^2 = (\frac{3}{2}\pi-1)\bar{z}^2$.

The correlation coefficients ρ_{xz} and ρ_{yz} have the properties that

$$\lim_{\zeta\to 0} \rho_{xz} = \lim_{\xi\to 0} \rho_{yz} = 0 \tag{3.24}$$

This corresponds to the case where no correlation exists between the position of the particle in the xz and yz planes.

3.5. Determination of the shearing parameter, F

In order to calculate the variables (ζ,ξ) from Eqs. (3.13) and (3.14), the shearing parameter F from (3.12) now has to be determined. For a neutral atmosphere, Chatwin (1968) investigated theoretically the along-wind dispersion of a puff of passive contaminant, released from a source near the ground. He found

$$\Sigma_x = 0.803\,\frac{u_* t}{k} \tag{3.25}$$

By setting $q = 1$ in Eq. (3.18), we have correspondingly for the skewed puff in a neutral atmosphere

$$\Sigma_x^2 = \sigma_x^2 + \zeta^2\bar{z}^2 \tag{3.26}$$

Substitution of ζ from Eq. (3.13) into (3.26) yields

$$\Sigma_x^2 = \sigma_x^2 + \left[\int_0^t (u_r\{\bar{z}(1+F)\} - u_r\{\bar{z}(1-F)\})d\tau \right]^2 \tag{3.27}$$

By use of the logarithmic character the mean wind profile $u_r(z)$ in the neutral case, the result after integration becomes

$$\Sigma_x^2 = \sigma_x^2 + \ln^2\left\{\frac{(1+F)}{(1-F)}\right\} \frac{u_*^2 t^2}{k^2} \tag{3.28}$$

By estimating σ_x^2 from Eq. (3.8) as $(0.22\ u_*t)^2$ and by substituting Eq. (3.25) for Σ_x^2, F is determined from the following equation:

$$(0.803)^2 = (0.22)^2 k^2 + \ln^2\left\{\frac{1+F}{1-F}\right\}, \tag{3.29}$$

from which we find F = 0.38.

The contribution to the total spread Σ_x from the spread at fixed height is, with the assumption $\sigma_x = 0.22\ u_*t$, indeed negligible relative to the contribution from the shearing of the puff $\ln\{(1+F)/(1-F)\}\ u_*t/k$ under neutral conditions.

Turning now to the case of a very stable atmosphere, where the wind shear $S = d\bar{u}_r/dz$ can be considered to be constant with height to a good approximation. The theory of Corrsin (1959) yields, in this case, the shear-induced spread in an unbound atmosphere:

$$\Sigma_x^2 = \frac{1}{3} S^2\ \Sigma_z^2 t^2 \tag{3.30}$$

The previous case of a neutral atmosphere proved that σ_x was small relative to the contribution from the shearing of the puff. Since the shearing of the puff in the stable atmosphere is even more pronounced at the same time as the spread σ_x diminishes, we can neglect the contribution of σ_x^2 to Σ_x^2 in Eq. (3.27). From Eqs. (3.18) and (3.20) we then have approximately that $\Sigma_x^2 \simeq \zeta^2\Sigma_z^2$. For a very stable atmosphere we also have from

Eqs. (2.18) and (2.19) that $u_r(z) \approx 4.7\ u_* z/(kL)$ and hence $S = 4.7\ u_*/(kL)$. With this, Eq. (3.13) becomes

$$\zeta = \frac{2FS}{\bar{z}(t)} \int_0^t \bar{z}(t')dt' \tag{3.31}$$

In the very stable atmosphere we found that $\bar{z}(t)$ is proportional to $\sqrt{t}$, so in this case we have

$$\xi = \frac{4}{3} FSt \tag{3.32}$$

The resulting streamwise spread of the skewed puff consequently becomes

$$\Sigma_x^2 = \left(\frac{4}{3} FS\ \Sigma_z t\right)^2 \tag{3.33}$$

and comparison with Eq. (3.30) yields the value $F = 0.43$; this is to be compared with the previous result for the neutral case, $F = 0.38$.

The slightly different values found for the constant F may be attributed to the following: Corrsin's model (Eq. 3.30) applies to the case of an unbound atmosphere, whereas Eq. (3.25) is for a ground level release. Consequently, the vertical spread in the latter case is confined to the halfplane above ground level only. Turning finally to the case of a very unstable atmosphere, we expect the influence on Σ_x from the shearing of the puff to be negligible relative to the spread σ_x since the mean wind profile here is approximately constant with height and the parameter F is of no importance in this case.

In conclusion, the above analysis suggest a value of the shearing parameter F close to 0.4 for use in models as a compromise for the broad range of stabilities discussed.

4. APPLICATIONS

The behaviour of the skewed puff with variable atmospheric stability is best illustrated by examples. Three atmospheric conditions: stable, L = 100; neutral, L = ∞; and unstable, L = - 100 were selected and the horizontal puff spread estimated using $\sigma_x = \sigma_y = 0.22\ u_*t$. The following initial values were selected: $\bar{z}(0) = 0.01$ m and $\sigma_x(0) = \sigma_y(0) = 0.1$ m. The surface roughness z_o was taken equal to 0.1 cm and the surface stress u_* was assumed to be 0.2 m s^{-1}.

Using these values, the positions of the centroids $(\bar{x},\bar{z})$ of the clouds were evaluated from Eqs. (2.16) and (2.17) concurrently with the shape parameter q from Eqs. (2.13) and (2.14). Setting the shearing parameter F = 0.38, the skewing parameter ζ was also calculated concurrently on the basis of Eq. (3.13). The lateral shear and thereby ξ, on the other hand, was assumed to be zero.

The three-dimensional concentration distribution function, Eq. (3.15), describing the skewed puff is thereby specified as function of the travel time t, and Fig. 5 shows the iso-concentration curve going through the centroid $(\bar{x},\bar{z})$ at time t = 100 s, for the three different stabilities considered. The intention in drawing the five ellipses is to visualize the symmetry of the puff in horizontal planes at an arbitrary height. When looked at from above, these ellipses will be circles with centre position (x_c,y_c) given by $(\zeta z,o)$ and radus $r = \sigma_x \{2b^q(1-z/\bar{z})^q\}^{1/2}$ with $\sigma_x = \sigma_y$.

When a stable condition is changed through a neutral to an unstable one, the example shows that the mean height $\bar{z}$ of the cloud at fixed time increases, at the same time that the shape parameter q decreases. It is also evident from the figure that the contribution from the wind shear to the total horizontal spread Σ_x in this example is dominant over the spread at fixed height σ_x for all the three different stabilities considered. It can be concluded from the example that the spread σ_x yields a significant contribution to Σ_x in only a very unstable atmosphere.

The example seems also to suggest that the quantity Σ_x is approximatively constant over a broad range of stability around neutral. The specific results of the example are given in Table 1.

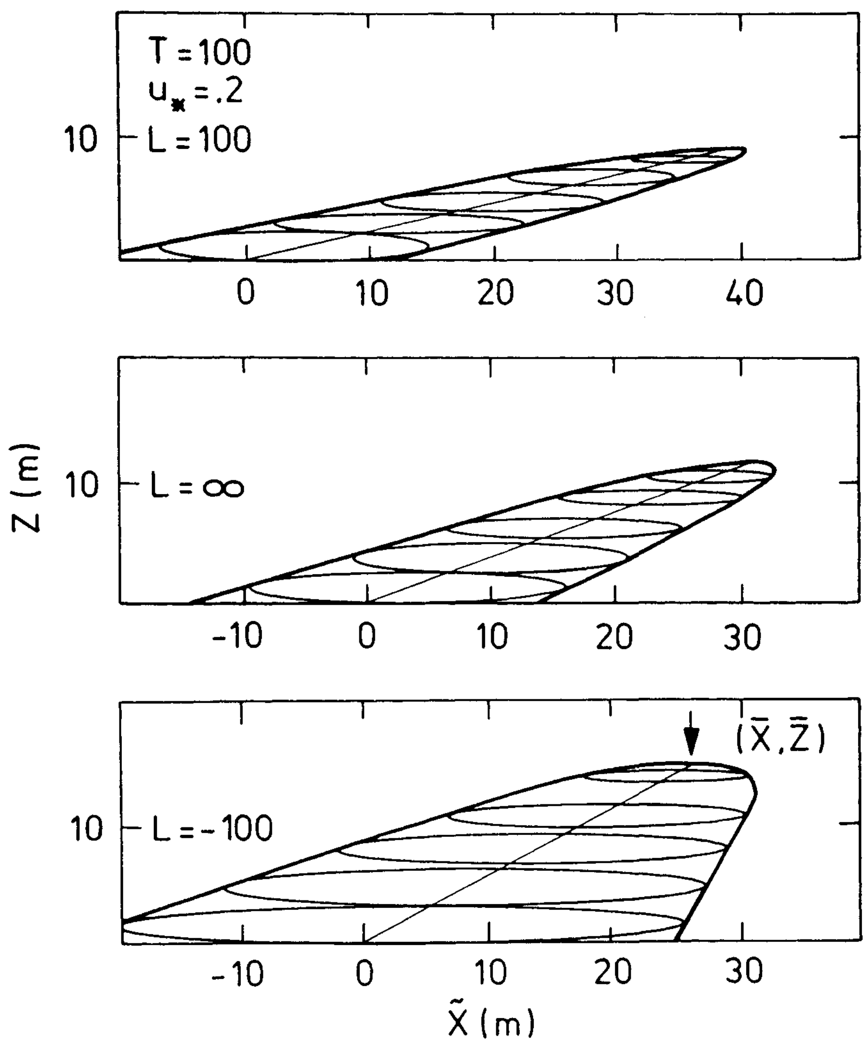

Fig. 5. Skewed puff at t = 100 s for three atmospheric conditions: stable (L = 100), neutral (L = ∞) and unstable (L = -100). Solid line shows the iso-concentration curve going through the centroid ($\bar{x}$,$\bar{z}$) in the vertical plane at y = 0. The five circles in each plot are drawn to envision the extension of the isoconcentration curve into the cross wind direction. Reference on the abscissa is to the coordinate system $\tilde{x}$ moving with the base of the cloud, as defined in Eq. (3.4), and z is the height above the ground.

Table 1. Example in Fig. 5 with $u_* = 0.2\ ms^{-1}$, $z_o = 0.01$ m, T = 100 s

Stab-ility	Skewing parameter	Mean wind speed (10 m)	Mean along wind distance	Mean height	Fixed height along wind spread	Total along wind spread	Total vertical spread	Shape parameter
L[m]	ζ	$\bar{u}_{10}[ms^{-1}]$	$\bar{x}[m]$	$\bar{z}[m]$	$\sigma_x[m]$	$\Sigma_x[m]$	$\Sigma_z[m]$	q
100	4.40	4.84	462	9.1	5.2	77.5	17.6	1.37
∞	2.73	4.61	457	11.8	9.7	63.0	22.8	1.00
-100	1.82	4.47	453	15.0	9.9	53.0	28.8	0.65

5. CONCLUSION

A model for the spread of a ground-level released puff of passive contaminant in a diabatic stratified surface layer has been developed for use in predicting the pollutant concentration in connection with a numerical puff model, where a series of puffs are emitted successively from the source.

The following three-dimensional, normalized concentration distribution function of individual puffs has been proposed:

$$C(\tilde{x},\tilde{y},\tilde{z}) =$$

$$\frac{a}{2\pi\sigma_x\sigma_y\bar{z}} \exp\left[-\frac{1}{2}(\tilde{x}-\zeta\tilde{z})^2/\sigma_x^2 - \frac{1}{2}(\tilde{y}-\zeta\tilde{z})^2/\sigma_y^2 - \left(\frac{b\tilde{z}}{\bar{z}}\right)^q\right] \tag{5.1}$$

where the two parameters (ζ,ξ) account for the shearing effect of the vertical wind velocity gradient. Their values are calculated by tagging the position of two tracer particles, z_1 and z_2, displaced by the distance $F\bar{z}$ about the mean height $\bar{z}$. The value of the constant F has been determined (0.38) in order that the total horizontal spread of the cloud equals the theoretical predictions of the spread that results as a consequence of the interaction of shear and vertical diffusivity under neutral and very stable atmospheric conditions. The vertical concentration distribution

$$C_V(z) = \iint C(\tilde{x},\tilde{y},\tilde{z})d\tilde{x}d\tilde{y} = a/\bar{z}\exp(-b\tilde{z}/\bar{z})^q , \tag{5.2}$$

which is known to satisfy the diffusion equation exactly with a power-law representation of the vertical eddy diffusivity, has been shown to be applicable also from numerical solutions of the diffusion equation (2.7), when $\bar{z}$ is determined by the approximation

$$\frac{d\bar{z}}{dt} = K_z(\bar{z}/L)/\bar{z} \qquad (5.3)$$

and the shape parameter q is determined by

$$q = 2 - d\log K_z/d\log z, \quad \text{with } z = \bar{z} \,. \qquad (5.4)$$

A numerical example seems to indicate that the total horizontal spread of the cloud Σ_x, at the fixed travel time t = 100 s, is approximately constant over a broad range of the atmospheric stability. In contrast, the mean height $\bar{z}$ and the cloud shape parameter q are found to be strongly influenced by changes in atmospheric stability.

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